Low Rank Approximation-based Quadrature for Fast Evaluation of Multi-Particle Integrals

Sandia National Laboratories

Univ. of Illinois at Urbana-Champaign

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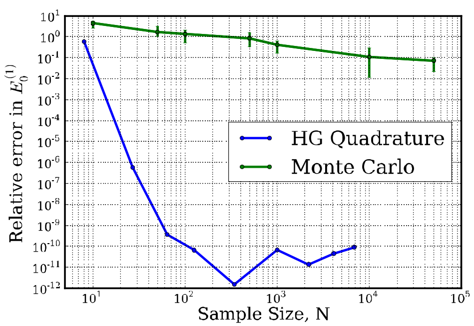
Objectives

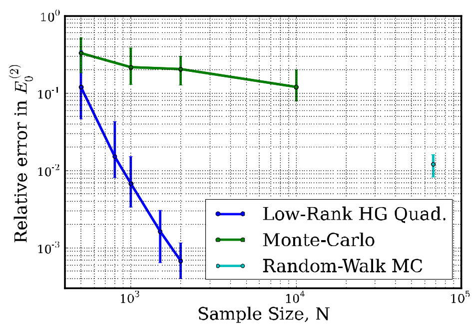
- Develop efficient integration methods for high-dimensional integrals arising in quantum chemistry
- Explore the utility of quadrature methods and low-rank tensor approximations for integration efficiency and scalability gains
- Evaluate the integration performance with respect to the number of function evaluations (chemistry computations) compared to the state-of-the-art Monte-Carlo methods

Impact

- Provides a potentially scalable approach for a wide range of high-dimensional quantum chemistry calculations
- Enables efficient energy level computations in anharmonic vibrational theory
- Allows rigorous uncertainty quantification and predictive simulation improvements



Unisootropic sparse quadrature for the first-order energy correction $E_0^{(1)}$



Low-rank approximation-based quarature integration for the second-order energy correction $E_0^{(2)}$

Accomplishments

- Demonstrated the low-rank approximation based quadrature integration for water molecule as a proof-of-concept
- Improved the state-of-the-art by a few orders of magnitude for small molecules
- Developed a semi-automatic recipe for high-dimensional quantum chemistry integration with a controllable accuracy-vs-efficiency tradeoff
- Journal paper is in preparation

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